Effect of temperature on the initial yield stress of single crystal (*)

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A DISCUSSION is given of a thermodynamic technique to compute the variation of initial yield stress with temperature in uniaxially loaded single crystals. It assumes a sharp and thermodynamically reversible elastic-plastic boundary and the linear thermo-elasticity. The result is a differential equation $d\sigma_y/dT = -(1/2)\sigma_y/T$ for all crystal systems in which σ_y is the uniaxial yield stress and T the absolute temperature. It is believed that since plastic transition consists in the onset of the migration of defects such as dislocations, and is sensitive to structural inhomogeneities, the above equation is expressing the extent of the role, if any, played by reversible thermodynamic parameters in the variation of yield stress with temperature. The theoretical result was compared with measurements in several crystallographic systems.

1. Introduction

PLASTIC deformation of crystalline materials involves the motion of lattice defects such as dislocations through crystal grains or round their boundaries. Twinning provides an exception, but it can supply only a limited amount of plastic deformation. According to the dislocation theory of plasticity in metals, the yield stress which signifies the beginning of significant sliding of dislocations is governed by several temporarily energy storing processes: (a) Interaction of dislocations, (b) Peierls-Nabarrow forces, (c) Local disarrangements of structure, (d) Pinning of dislocations by dissolved atom, known as Cottrell mechanism, etc. Therefore the temperature dependence of yield stress has been interpreted mostly from the standpoint of activation energies involving various temperature sensitive dislocation mechanisms. For example, FISHER [1] showed that in the case of Cottrell mechanism, the yield stress is inversely proportional to the temperature, and that the result is in agreement with the experimental data concerning Mo and Fe. Some of the other equations which have been proposed are 1) $\sigma_Y = a - bT^{1/2}$ [2, 3], 2) $\sigma_Y = a - bT$ [4–7], 3) $\sigma_Y = a + b/T$ [8], 4) $\ln \sigma_Y = a + b/T$ [9], where σ_Y is the yield stress, T the temperature, a and b are constants. In general, each of these equations is restricted to certain materials and over a limited temperature range.

There are, however, other athermal effects which influence the effect of temperature on the initial yield stress. In particular, the variation of elastic moduli is a well known example [10]. Therefore, the aim of this paper is to present an approximate method of computing the variation of the yield stress with temperature on the basis of a purely thermodynamic approach. Th is approachis conceived in part to test the validity of a widely accepted contemporary continuum view [11–13] that there is always an elastically strained lattice

imbedded in every plastically deformed state, and that this elastic state is inherently revers-
ible and can be recovered by suitable reversible processes. However in order to concentrate
on essentials, the discussion will be limited to the variation of the initial yield stress of
uniaxially loaded single crystals in simple tension. And the equilibrium equation of state
will be confined to that of linear infinitesimal thermo-elasticity.

2. Elastic-plastic boundary and a reversible loop

Experimentally speaking, there are several ways to identify the elastic-plastic transition,
but here is simply assumed the existence of a sharp boundary between the elastic and the
plastic domains in the stress-strain-temperature space for uniaxially loaded crystals, Fig. 1.
Then in order to characterize the boundary, we introduce reversible isothermal and adia-
batic loadings starting from a common origin, 0, an unloaded state at temperature T, as
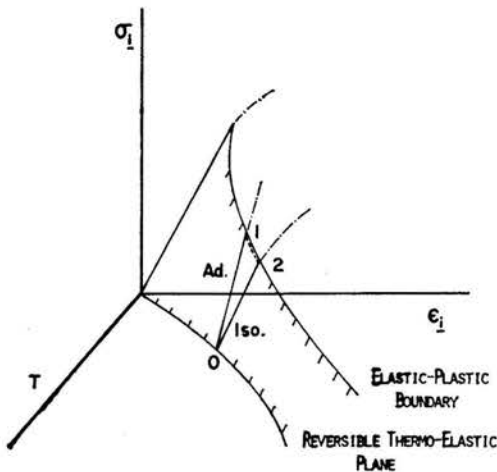shown in Figs. 1 and 2. They intercept the boundary at states 1 and 2. Since in normal
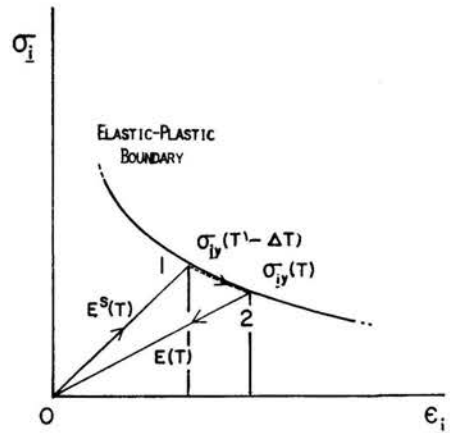

FIG. 1. Reversible loop.

FIG. 2. Linear approximation of the reversible
loop at T.

crystals simple tension produces a very small temperature drop, the adiabatic loading
path will lie above the isothermal one, provided that the yield stress decreases as the
temperature of specimens increases.

Obviously, a loop 0120 is formed by the isothermal and adiabatic processes and the
elastic-plastic boundary. However, if the elastic-plastic boundary is replaced by a reversible
path represented by a broken line in Fig. 2, the resulting loop consists of entirely revers-
ible paths. Hence one complete loop must restore the original value of internal energy
at T,

$$\oint_{0\dot{1}20} dU = \int_{0\dot{1}20} \left(\frac{\sigma_{ij} d\varepsilon_{ij}}{\varrho_0} + T dS \right) = 0,$$

where ϱ_0 is the density, U and S are the specific internal energy and the entropy per unit mass, and σ_{ij} and ε_{ij} are stress and strain components, respectively.

Then one observes that, since the area of a loop is finite, the slope of the boundary must be reflected in the difference between the isothermal and the adiabatic deformations. A quantitative relation may be revealed by evaluating the internal energy change along each path.

Path 01. Since there is no entropy change along the path,

$$(2.1) \qquad \int_0^1 dU = \int_0^1 \left(\frac{\sigma_{ij} d\varepsilon_{ij}}{\varrho_0} \right)_s.$$

If the linear-thermo-elasticity is assumed, the Eq. (2.1) reduces to

$$(2.2) \qquad \int_0^1 dU = \sigma_{iY}^2 (T - \Delta T)/2\varrho_0 E^s,$$

where σ_{iY} signifies the tensile yield stress in a loading direction $\underline{i}$, ΔT the small temperature drop between states 1 and 2, E^s the adiabatic Young's modulus along the path 0-1.

Path 12. The internal energy change involves both work and entropy terms. However, since the adiabatic temperature drop ΔT is ordinarily very much smaller than T (this will be seen later), the path integral may be approximated by the following expressions,

$$(2.3) \qquad \int_1^2 dU = \int_1^2 \sigma_{iY} d\varepsilon_i/\varrho_0 + \int_1^2 T dS = \frac{1}{2\varrho_0}[\sigma_{iY}(T) + \sigma_{iY}(T - \Delta T)] [\sigma_{iY}(T)/E$$

$$- \sigma_{iY}(T - \Delta T)/E^S] + \int_1^2 T \left[\left(\frac{\partial S}{\partial T} \right)_{\sigma_{ij}} + \left(\frac{\partial S}{\partial \sigma_i} \right)_T \frac{d\sigma_i}{dT} \right] dT = \frac{1}{2\varrho_0}[\sigma_{iY}(T)$$

$$+ \sigma_{iY}(T - \Delta T)] [\sigma_{iY}(T)/E - \sigma_{iY}(T - \Delta T)/E^S] + \Delta T \left[C + \frac{T a_{ii}}{\varrho_0} \left(\frac{d\sigma_{iY}}{dT} \right) \right],$$

where E is the isothermal Young's modulus for the axis $\underline{i}$, and the following equilibrium relations are used,

$$T \left(\frac{\partial S}{\partial T} \right)_{\sigma_{ij}} = C_\sigma = \text{a specific heat,}$$

$$\varrho_0 \left(\frac{\partial S}{\partial \sigma_{ij}} \right)_R = \left(\frac{\partial \varepsilon_{ij}}{\partial T} \right)_{\sigma_{ij}} = a_{ij} = \text{thermal expansion coefficients.}$$

Path 20. Since the path is isothermal at T,

$$(2.4) \qquad \int_2^0 dU = -\frac{\sigma_{iY}^2(T)}{2\varrho_0 E} - T[S(\sigma_{iY}, T) - S(0, T)].$$

If a_{ii} is independent of σ_i, then it is found that by use of Taylor's expansion of S

$$(2.5) \qquad \int_2^0 dU = -\frac{\sigma_{iY}^2(T)}{2\varrho_0 E} - \frac{T}{\varrho_0} a_{ii} \sigma_{iY}(T).$$

Now combining the Eqs. (2.2), (2.4), and (2.5), one obtains

$$(2.6) \qquad \frac{\sigma_{iY}(T)\sigma_{iY}(T-\Delta T)}{2\varrho_0}\left(\frac{1}{E}-\frac{1}{E^s}\right)+\left[C_\sigma+\frac{T}{\varrho_0}\alpha_{ii}\left(\frac{d\sigma_{iY}}{dT}\right)\right]\Delta T-\frac{T}{\varrho_0}\alpha_{ii}\sigma_{iY}(T)=0.$$

In order to simplify the equation, we need ΔT and $\left(\dfrac{1}{E}-\dfrac{1}{E^s}\right)$. According to THURSTON [14], adiabatic temperature changes are given by

$$dT = -\frac{T}{\varrho_0 C_\varepsilon}\lambda_{ij}d\varepsilon_{ij}^s,$$

where

$$\lambda_{ij}=\varrho_0\left(\frac{\partial S}{\partial \varepsilon_{ij}}\right)_T=\alpha_{ln}C_{lnij}^T=\alpha_{ln}C_{ijln}^T, \qquad C_\varepsilon=T\left(\frac{\partial S}{\partial T}\right)_{\varepsilon_{ij}},$$

$$C_{ijkm}^T=\left(\frac{\partial \sigma_{ij}}{\partial \varepsilon_{km}}\right)_T, \qquad d\varepsilon_{ij}^s=s_{ijkm}^s d\sigma_{km}, \qquad s_{ijkm}^s=\left(\frac{\partial \varepsilon_{ij}}{\partial \sigma_{km}}\right)_S.$$

Hence the magnitude of temperature drop ΔT for the uniaxial stress $\sigma_{iY}(T-\Delta T)$ is

$$(2.7) \qquad \Delta T=\frac{T}{\varrho_0 C_\varepsilon}\alpha_{ln}C_{lnkm}^T s_{kmii}^s \sigma_{iY}(T).$$

For steel, ΔT is about 0.125°C when $T = 274.7°K$ and $\sigma = 10^9$ dynes/cm².

The difference $(1/E-1/E^s)$ can be determined by use of adiabatic and isothermal compliance coefficients,

$$1/E = s_{iiii}^T, \qquad 1/E^s = s_{iiii}^s$$

and an identity relation

$$s_{ijkm}^T - s_{ijkm}^s = T\alpha_{ij}\alpha_{km}/\varrho_0 C_\sigma,$$

where $s_{ijkm}^T = (\partial \varepsilon_{ij}/\partial \sigma_{km})_T$.

The result is

$$(2.8) \qquad \left(\frac{1}{E}-\frac{1}{E^s}\right)=T\alpha_{ii}^2\varrho_0 C_\sigma.$$

Finally, the substitution of the Eqs. (2.7) and (2.8) into (2.6) yields

$$(2.9) \qquad \begin{aligned}\frac{d\sigma_{iY}}{dT} &= -1/2\left(\frac{C_\varepsilon}{C_\sigma}\right)\frac{\alpha_{ii}}{\alpha_{lm}C_{lmop}^T s_{opii}^s}\left(\frac{\sigma_{iY}(T)}{T}\right)\\ &\quad -\left(\frac{\varrho_0 C_\sigma}{T\alpha_{ii}}\right)\left[1-\frac{C_\varepsilon}{C_\sigma}\frac{\alpha_{ii}}{\alpha_{lm}C_{lmop}^T s_{opii}^s}\frac{\alpha_{iY}(T)}{\sigma_{iY}(T-\Delta T)}\right].\end{aligned}$$

We see in the above equation that the derivative on the left-hand side comes from the approximation used for Path 12 in the Eq. (2.3), and that it is the only term that reflects the slope of the elastic-plastic boundary between T and $T-\Delta T$. Therefore, in view of (2.7) the ratio $\sigma_{iY}(T)/\sigma_{iY}(T-\Delta T)$ in the last term can be approximated by one. Then we find

$$(2.10) \qquad \frac{d\sigma_{iY}}{dT}=-\frac{1}{2}\frac{C_\varepsilon}{C_\sigma}\frac{\alpha_{ii}}{\alpha_{lm}C_{lmop}^T s_{opii}^s}\left(\frac{\sigma_{iY}}{T}\right)-\frac{\varrho_0 C_\sigma}{T\alpha_{ii}}\left[1-\frac{C_\varepsilon}{C_\sigma}\frac{\alpha_{ii}}{\alpha_{lm}C_{lmop}^T s_{opii}^s}\right].$$

This result can be further simplified by the following relation [15]

(2.11)

$$\lambda_{ij} = \alpha_{km} C_{kmij}^T = \frac{C_\varepsilon}{C_\sigma} \alpha_{km} C_{kmij}^s,$$

$$C_{ijkm}^s s_{kmln}^s = 1/2(\delta_{il}\delta_{jn} + \delta_{in}\delta_{jl}),$$

where $C_{kmij}^s = (\partial \sigma_{km}/\partial \varepsilon_{ij})_s$.

Then the substitution produces a simple result,

$$\frac{d\sigma_{iY}}{dT} = -1/2\left(\frac{\sigma_{iY}}{T}\right),$$

or

(2.12)

$$\sigma_{iY} T^{1/2} = \text{constant}.$$

3. Discussions

Contrary to our experience, the Eq. (2.12) predicts an infinite yield stress at $T = 0$. This singularity results from the fact that at $T = 0$, the method breaks down due to the third law of thermodynamics (Nernst law), that is, there is no difference between isothermal and adiabatic processes at the absolute zero. Otherwise within the limit of the approximation involved, the Eq. (2.12) determines the equilibrium effect of temperature on the initial yield stress of single crystals.

Figures 3–6 compare the curves $\sigma_Y T^{1/2} = \text{constant}$ with experimental data in various crystal classes. The Eq. (2.12) may be a result of oversimplification, but the simple analysis appears to be adequate in representing a reversible change in the yield stress.
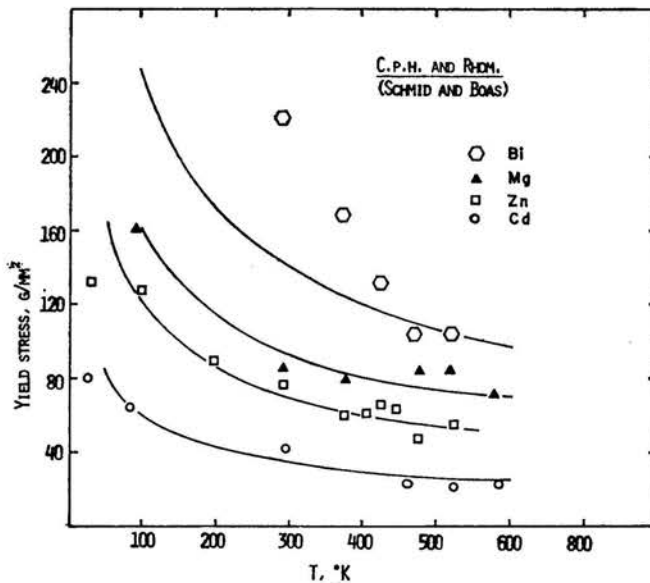

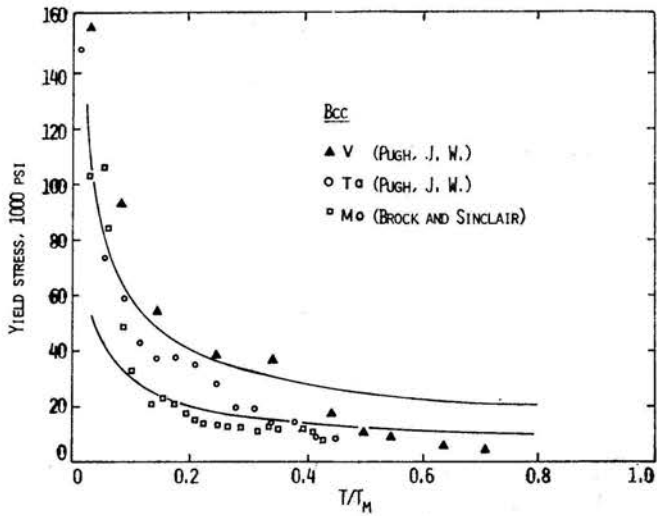FIG. 3. Effect of temperature on the initial yield stress.

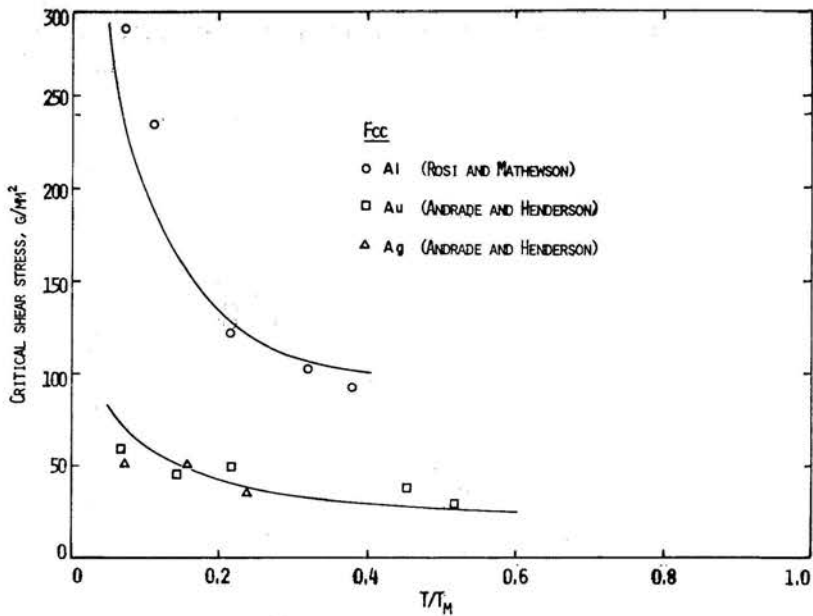FIG. 4. Yield stress versus homologous temperature T/T_M.

FIG. 5. Cristal resolved shear stress versus homologous temperature T/T_M.
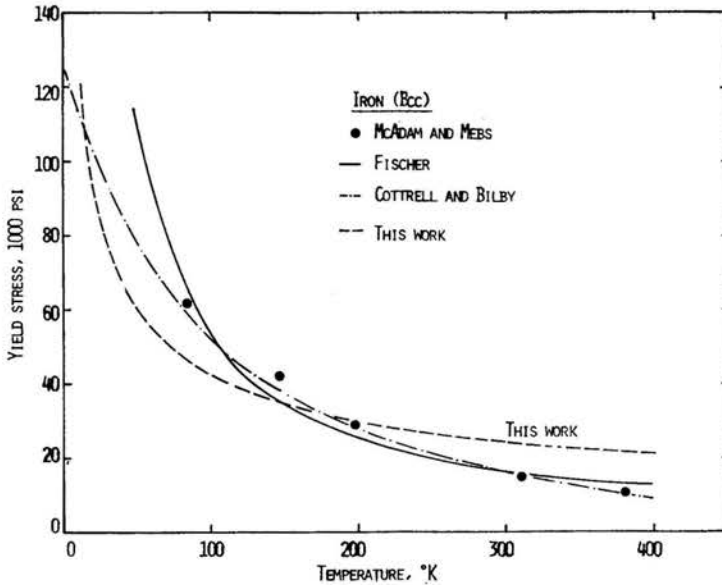
FIG. 6. Yield stress versus temperature for iron (References are given in Ref. [1]).

At low temperatures, metals with a *bcc* structure show a stronger temperature dependence than the Eq. (2.12). This is not unexpected, because there are other effects in the yield stress which are structure sensitive and cannot be accounted for by a reversible thermodynamics. Such effects must be related to the detailed nature of dislocation structures in crystals and their irreversible motions.

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